

On nonsingular potentials of Cox-Thompson inversion scheme

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Abstract

We establish a condition for obtaining nonsingular potentials using the CoxThompson inverse scattering method with one phase shift. The anomalous singularities of the potentials are avoided by maintaining unique solutions of the underlying ReggeNewton integral equation for the transformation kernel. As a by-product, new inequality sequences of zeros of Bessel functions are discovered.

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1 Introduction

The Regge-Newton integral equation of the Cox-Thompson method [1] for the transformation kernel reads as

$$K(x, y) = g(x, y) - \int_0^x dt t^{-2} K(x, t) g(t, y), \quad x \geq y, \quad (1)$$

with the input symmetrical kernel defined as

$$g(x, y) = \sum_{l \in S} \gamma_l u_l(x_{<}) v_l(x_{>}), \quad \begin{aligned} x_{<} &= \min(x, y), \\ x_{>} &= \max(x, y). \end{aligned} \quad (2)$$

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Here u_l and v_l means, respectively, the regular and irregular Riccati-Bessel functions defined as $u_l(x) = \sqrt{\frac{\pi x}{2}} J_{l+\frac{1}{2}}(x)$, $v_l(x) = \sqrt{\frac{\pi x}{2}} Y_{l+\frac{1}{2}}(x)$, and the explicit expression holds for the γ_l numbers:

$$\gamma_l = \frac{\prod_{L \in T} [l(l+1) - L(L+1)]}{\prod_{l' \in S, l' \neq l} [l(l+1) - l'(l'+1)]}, \quad l \in S, \quad (3)$$

with $|S| = |T| < \infty$, $T \subset (-1/2, \infty)$, $S \subset (-1/2, \infty)$ and $S \cap T = \emptyset$ [1, 2].

Let Ω denote the set of zeros of the determinant

$$D(x) = \det(C(x)) \quad (4)$$

with

$$[C(x)]_{lL} = \frac{u_L(x)v'_l(x) - u'_L(x)v_l(x)}{l(l+1) - L(L+1)}. \quad (5)$$

In Ref. [2] it is proved that equation (1) is uniquely solvable for $x \in \mathbb{R}^+ \setminus \Omega$ and the elements of Ω are isolated points. Therefore the continuous solution of equation (1) (if it exists) is unique.

In Ref. [3] it has been shown that $tq(t)$ is not integrable near $\tilde{x} \in \Omega$. Therefore the potential $q(x) := -\frac{2}{x} \frac{d}{dx} \frac{K(x, x)}{x}$ corresponding to the Schrödinger equation has poles of order (at least) 2 at these isolated points \tilde{x} . Such potentials are not in $L_{1,1}(0, \infty)$ and we call them singular potentials.

To get non-singular potentials by the Cox-Thompson method is thus in an intimate connection with the uniqueness of solution of equation (1). From now on the treatment is restricted to the one-term limit, i.e., to the case when $|S| = |T| = 1$. Such a case represents a natural first step compared to the uniqueness solution of the CT method with finite number of phase shifts. Also, the one phase shift case is closely related to the phenomenon of quantum resonance scattering (when the resonance-like enhancement of the total cross section is mainly determined by a single partial wave) or the Ramsauer-Townsend effect (when the electron-atom interaction is governed mainly by the p -wave phase shift) [4].

In the one-term limit, the numerator of equation (5) becomes the Wronskian

$$W_{Ll}(x) = u_L(x)v'_l(x) - u'_L(x)v_l(x) = \frac{\pi x}{2} \left(J_{L+\frac{1}{2}}(x)Y'_{l+\frac{1}{2}}(x) - J'_{L+\frac{1}{2}}(x)Y_{l+\frac{1}{2}}(x) \right). \quad (6)$$

To ensure a unique solution of the Regge-Newton integral equation (1), we shall establish a condition for $W_{Ll}(x) \neq 0$, $x \in (0, \infty)$. This is also the condition for constructing a non-singular potential $q(x)$, $x \in (0, \infty)$ at the one-term level $|S| = |T| = 1$.

2 Condition for constructing non-singular potentials from one specified phase shift

Let $S = \{l\}$ and $T = \{L\}$, $L \neq l$. In order to get a potential that belongs to the class $L_{1,1}(0, \infty)$ we shall prove the next statement.

Theorem 2.1. $W_{Ll}(x) \neq 0, \quad x \in (0, \infty) \iff 0 < |L - l| \leq 1.$

Proof. First we prove that there exists $x > 0$ such that $W_{Ll}(x) = 0$ if $|L - l| > 1$. Let $1 + 4k < l - L < 3 + 4k$ with $k \in \mathbb{Z}$. Then the different sign of the Wronskian at the origin $W_{Ll}(x \rightarrow 0) = x^{L-l} \left[\frac{2^{l-L-1}(L+l+1)\Gamma(l+\frac{1}{2})}{\Gamma(L+\frac{3}{2})} + O(x^{2l+1}) \right] > 0$ and at the infinity $W_{Ll}(x \rightarrow \infty) = \cos \left[(l - L) \frac{\pi}{2} \right] < 0$ clearly signals the existence of at least one zero position \tilde{x} for which $W_{Ll}(\tilde{x}) = 0$ because of the continuity of $W_{Ll}(x)$.

For the uncovered region of $3 + 4k < l - L < 5 + 4k$ with $k \in \mathbb{Z} \setminus \{-1\}$ we shall use the standard notation for the n th zeros $j_{L+\frac{1}{2},n}, j'_{L+\frac{1}{2},n}, y_{l+\frac{1}{2},n}, y'_{l+\frac{1}{2},n}$ of the Bessel functions $J_{L+\frac{1}{2}}(x), J'_{L+\frac{1}{2}}(x), Y_{l+\frac{1}{2}}(x), Y'_{l+\frac{1}{2}}(x)$. Let now $l < L$. We term *regular* sequence of zeros if the following interlacing holds for the n th and $(n+1)$ th zeros: $y_{l+\frac{1}{2},n} < j_{L+\frac{1}{2},n} < y_{l+\frac{1}{2},n+1} < j_{L+\frac{1}{2},n+1}$. It is a simple matter to see that the local extrema of $W_{Ll}(x)$ within the interval $y_{l+\frac{1}{2},n} < x < j_{L+\frac{1}{2},n+1}$ possess the same sign in case of regular sequence interlacing. This is because at the extremum positions $y_{l+\frac{1}{2},n}$ and $j_{L+\frac{1}{2},n}$ of $W_{Ll}(x)$ the Wronskian simplifies to

$$W_{Ll}(x_n) = \begin{cases} \frac{\pi x}{2} J_{L+\frac{1}{2}}(x_n) Y'_{l+\frac{1}{2}}(x_n) & \text{if } Y_{l+\frac{1}{2}}(x_n) = 0, x_n = y_{l+\frac{1}{2},n} \\ -\frac{\pi x}{2} J'_{L+\frac{1}{2}}(x_n) Y_{l+\frac{1}{2}}(x_n) & \text{if } J_{L+\frac{1}{2}}(x_n) = 0, x_n = j_{L+\frac{1}{2},n}. \end{cases} \quad (7)$$

Now, in case of any deviation from this regular sequence, e.g., when an *irregular* sequence $y_{l+\frac{1}{2},n} < y_{l+\frac{1}{2},n+1} < j_{L+\frac{1}{2},n}$ is first encountered at a particular $n = 1, 2, \dots$, one gets different signs for the two consecutive extrema of the Wronskian at $y_{l+\frac{1}{2},n}$ and $y_{l+\frac{1}{2},n+1}$, respectively. This assumes the appearance of a zero position of $W_{Ll}(x)$ within the region $y_{l+\frac{1}{2},n} < x < y_{l+\frac{1}{2},n+1}$. In summary, observing regular sequences of interlacing for all $n > 0$ is equivalent to the absence of roots of $W_{Ll}(x)$. To see that in the considered region such deviation from the regular sequence interlacing happens we present the following argument. Let $L' < L$ such that $1 + 4k < l - L' < 3 + 4k$. For $W_{L'l}$ the first deviation from the regular sequence takes place at some n' . It is easy to see that by increasing L' to L one cannot get a regular sequence and the first deviation will occur at some $n \leq n'$. Note that the case $L < l$ can be similarly treated.

Turning now to the most interesting domain of $0 < |L - l| \leq 1$, we consider again the case $l < L$ and the regular sequence of zero interlacing, $y_{l+\frac{1}{2},n} < j_{L+\frac{1}{2},n} < y_{l+\frac{1}{2},n+1} < j_{L+\frac{1}{2},n+1}$. As indicated above, its fulfillment ensures lack of root of the Wronskian: $W_{Ll}(x) \neq 0, x \in (0 < x < \infty)$. By noting that any n th zero of a Bessel function is a strictly growing function of the order it is sufficient to prove that $y_{k,n} < j_{k+1,n} < y_{k,n+1} < j_{k+1,n+1}$, holds for $k \in (0, \infty)$ and $n \in \mathbb{N} \setminus \{0\}$. The only unknown inequality here is that of $j_{k+1,n} < y_{k,n+1}$. To prove its validity we use the known intermediate relation $j'_{k,n+1} < y_{k,n+1}$. Therefore, proving $j_{k+1,n} < j'_{k,n+1}$ will suffice. Consider the known relation $J_{k+1}(j'_{k,n+1}) = \frac{k}{j'_{k,n+1}} J_k(j'_{k,n+1})$ which means that J_{k+1} and J_k have the same sign at $x = j'_{k,n+1}$. Now because of the interlacing

property $j_{k,1} < j_{k+1,1} < j_{k,2} < \dots$ and the limit $J_k(x \rightarrow 0) = 0^+ \forall k > 0$, this implies that the n th zero of $J_{k+1}(x)$ precedes the $(n+1)$ th zero of $J'_k(x)$, i.e. $j_{k+1,n} < j'_{k,n+1} < y_{k,n+1}$ which had to be proven. Note that the case $L < l$ can be similarly treated. \square

Corollary 2.2. *In case of $|S| = 1$, the Cox-Thompson inverse scattering scheme yields a potential of the class $L_{1,1}(0, \infty)$ iff the condition $0 < |l - L| \leq 1$ holds.*

In the course of the proof we obtained the following result of its own right:

Proposition 2.3. *Denoting the n th root of the Bessel functions $J_\nu(x)$, $Y_\nu(x)$, $J'_\nu(x)$, respectively, by $j_{\nu,n}$, $y_{\nu,n}$, $j'_{\nu,n}$ then the following inequality is valid for $\nu > 0$: $j_{\nu+1,n} < j'_{\nu,n+1}$.*

This proposition adds two new inequality sequences to the known ones (see e.g. Ref. [5]): $j_{\nu,n} < j_{\nu+1,n} < j'_{\nu,n+1} < j_{\nu,n+1}$, and $j_{\nu+1,n} < y_{\nu,n+1}$.

3 Construction of potentials from one phase shift

One can construct a potential that possesses one specified phase shift δ_l ($|S| = 1$) by using the inversion scheme of Cox and Thompson [1, 6]:

$$q(x) = -\frac{2}{x} \frac{d}{dx} \frac{K(x, x)}{x}, \quad (8)$$

$$K(x, y) = \frac{l(l+1) - L(L+1)}{u_L(x)v'_l(x) - u'_L(x)v_l(x)} v_l(x)u_L(y), \quad (9)$$

$$\tan(\delta_l - l\pi/2) = \tan(-L\pi/2). \quad (10)$$

Relation (10) gives $L = l - \frac{2}{\pi}\delta_l + 2n$, $n \in \mathbb{Z}$. For $\delta_l \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ the Corollary results in the choice of $n = 0$. Therefore, for any δ_l , there is only one, easily identifiable non-singular potential and an infinite number of singular potentials that the Cox-Thompson method can produce.

For an example let us choose $l = 0$ and $\delta_0 = 0$. In this case equation (10) yields $L = 2n$, $n \in \mathbb{Z}$. $L = 0$ ($n = 0$) is not permitted by the assumption $S \cap T = \emptyset$, however in order to get a non-singular potential one may replace this $L = 0$ by L_n with $\lim_{n \rightarrow \infty} L_n = 0$. Using equation (9) one gets at $l = 0$ and $L = L_n$

$$K_n(x, x) = \frac{-L_n(L_n + 1)}{1 + \varepsilon_n^1} (v_0(x)u_0(x) + \varepsilon_n^2). \quad (11)$$

Since $u_L(x)v'_l(x) - u'_L(x)v_l(x)$ and $v_l(x)u_L(x)$ are continuous in L and $u_l(x)v'_l(x) - u'_l(x)v_l(x) = 1$, $\forall l$, $\lim_{n \rightarrow \infty} \varepsilon_n^{1,2} = 0$ holds. Thus $\lim_{n \rightarrow \infty} q_n(x) \equiv 0$ for $x > 0$. This is the physical solution. (See Fig. 1.)

Now let $l = 0$ and $L = 2$. By the Corollary we cannot get an integrable potential in this case because $|l - L| > 1$ (see Fig. 1). In Ref. [7] it has been shown explicitly that equation (1) is not uniquely solvable at some x for this case. However, while Ref. [7] suggests that this fact makes the Cox-Thompson scheme

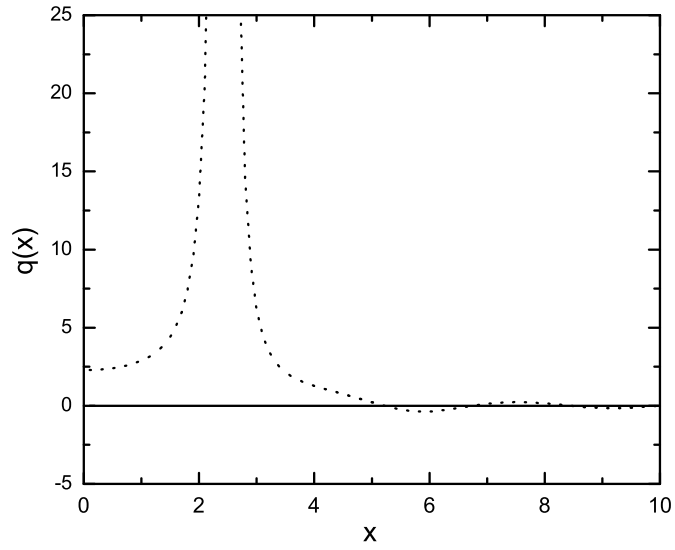


Figure 1: Nonsingular (full line) and singular (dotted line) potentials yielded by $\delta_{l=0} = 0$ with $L \rightarrow 0$, and $L = 2$.

useless, in this paper we have shown that in order to get an integrable potential, the choice $L = 2$ is not permitted because the set Ω is not empty. On the other hand, equation (10) and the Corollary provide a one-to-one correspondence between the phase shift and the L parameter of the Cox-Thompson method at the one-term level. This correspondence has the property that the potential constructed from L belongs to $L_{1,1}(0, \infty)$ and possesses the specified phase shift.

In Fig. 2 we add examples of the construction of an unique potential in $L_{1,1}$ in the case of non-trivial phase shifts. Subfigure Fig. 2a shows the potentials for zero angular momentum with $\delta_{l=0} = 0.780$ corresponding to $L = -0.497$ which is permitted by the Corollary (nonsingular case, full line) and $L = -0.497 + 2$ which violates the Corollary (one-singularity case, dotted line). Subfigure Fig. 2b shows the potentials for the p -wave phase shift $\delta_{l=1} = 1.50$ corresponding to $L = 0.045$ [permitted by the Corollary (nonsingular case, full line)] and $L = 0.044 + 4$ [violating the Corollary (two-singularity case, dotted line)]. We note that the second singularity of the dotted curve in Fig. 2b lies out of the region shown and, as expected from the *Proof*, the singular potentials in Fig. 2a and 2b have one and two locally non-integrable region(s) corresponding to $1 < |l - L| < 3$ and $3 < |l - L| < 5$, respectively.

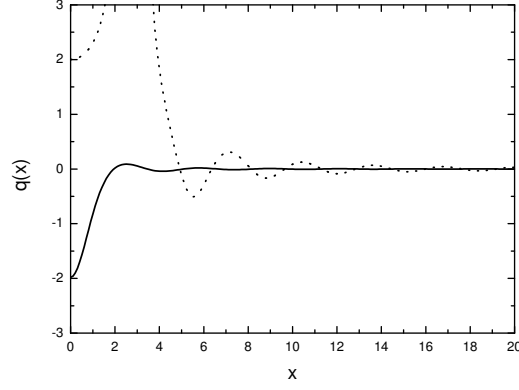
Applications (see Refs. [6, 8, 9, 10, 11, 12]) of the Cox-Thompson scheme for $|S| > 1$ suggest the existence of a connection similar to the Corollary of Section 2 that specifies one nonsingular potential out of the possible infinite singular solutions. However such a theorem has, as yet, not been proven.

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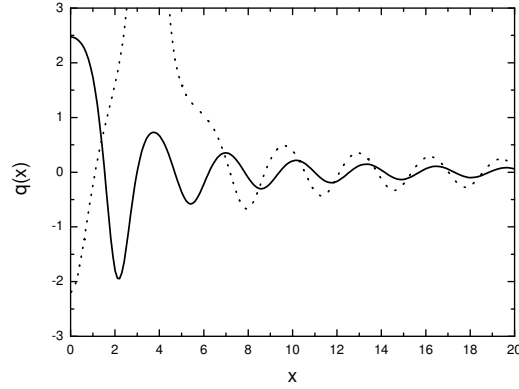
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References

- [1] J. R. Cox and K. W. Thompson, *J. Math. Phys.* **11**, 805, (1970).
- [2] J. R. Cox and K. W. Thompson, *J. Math. Phys.* **11**, 815, (1970).
- [3] K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer, New York, 1977), pp. 187-188.
- [4] B. H. Bransden, *Atomic Collision Theory* (The Benjamin/Cummings Publishing Company, London, 1983).
- [5] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1972), pp. 360-371.
- [6] B. Apagyi, Z. Harman and W. Scheid, *J. Phys. A: Math. Gen.* **36**, 4815, (2003).



(a)



(b)

Figure 2: Nonsingular (full line) and singular (dotted line) potentials yielded by nontrivial phase shifts. (a) $\delta_{l=0} = 0.780$ with $L = -0.497$ (full line) and $L = -0.497 + 2$ (dotted line); (b) $\delta_{l=1} = 1.50$ with $L = 0.045$ (full line) and $L = 0.045 + 4$ (dotted line, see text).

- [7] A. G. Ramm, *Applic. Anal.* **81**, 833, (2002); A. G. Ramm, *Mod. Phys. Lett. B* **22**, 2217, (2008).
- [8] O. Melchert, W. Scheid and B. Apagyi, *J. Phys. G* **32**, 849, (2006).
- [9] B. Apagyi W. Scheid, O. Melchert and D. Schumayer, *Nuclear Physics A* **790**, 767c, (2007).

- [10] D. Schumayer, O. Melchert, W. Scheid and B. Apagyi, J. Phys. B: At. Mol. Opt. Phys. **41**, 035302, (2008).
- [11] T. Pálmai, M. Horváth and B. Apagyi, J. Phys. A: Math. Theor. **41**, 235305, (2008).
- [12] T. Pálmai, M. Horváth and B. Apagyi, Mod. Phys. Lett. B **22**, 2191, (2008).